

SPECTROSCOPIC STUDY OF METHYLGLYOXAL AND ITS HYDRATES : A GASEOUS PRECURSOR OF SECONDARY ORGANIC AEROSOLS.

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Secondary organic aerosols (SOA) have a significant effect on climate change. They are mainly produced in the atmosphere by oxidation of gaseous precursors. Fu et al.^a have suggested trans-methylglyoxal (MG) as a possible precursor of SOA in the cloud for its presence in large quantities in the atmosphere.

The characterization of SOAs precursors by laboratory spectroscopy allows providing elements for the understanding of the process of formation of these aerosols. For this purpose, we completed the existing pure rotational spectrum of MG in the 12-40 GHz range^b by new records in a supersonic jet in the 4-20 GHz range (FTMW) and at room temperature in the 150-500 GHz range (mm/submm-wave spectrometer).

The analysis was made with the support of quantum chemistry calculations (MP2/CBS and B98/CBS using the Gaussian 09 software). The adjustment of the spectroscopic parameters, taking into account the internal rotation related to the presence of a methyl group, was performed using the RAM36 code. The spectra have been reproduced at the experimental precision up to maximal values of J and K_a equal to 85 and 35, respectively.

The data obtained for the isolated molecule, both experimentally and theoretically, will allow the study of its hydrated complexes and, by comparison, will give access to (micro-) hydration properties. For this purpose, two stable complexes predicted by theoretical calculations will be studied.

^aT.- M. Fu et al., J. Geophys. Res., 113, (2008).

^bC.E. Dyltick-Brenzinger and A. Bauder, Chem. Phys. 30, 147 (1978).